Hybrid of Adaptive Response Surface methodology and Genetic Algorithm Monte Carlo Optimization method and Its Application in the Design of Moderator-Collimator for Accelerator based Thermal Neutron Radiography*

> Chen-Xiao Yang,^{1,2} Si-Ze Chen,^{1,2,†} Lian-Xin Zhang,² Chuan Peng,^{2,3} and Dan Xiao² ¹Anhui University, Hefei, Anhui, 230601, China ²Hefei Institutes of Physical Science, Chinese Academy of Sciences, Hefei, Anhui, 230031, China ³University of Science and Technology of China, Hefei, Anhui, 230026, China

> A new Monte Carlo (MC) neutronics optimization method named Hybrid of Adaptive Response Surface methodology and Genetic Algorithm Monte Carlo Optimization (HRG-MCO) is proposed to address the strong empirical dependence and low efficiency of global multi-parameter optimization in traditional neutronics design. HRG-MCO integrates the advantages of Response Surface Methodology (RSM) and Genetic Algorithm (GA). Specifically, neutron MC simulation results are iteratively utilized to adaptively construct an RSM model, ensuring the required accuracy. Subsequently, GA is employed to perform multi-parameter optimization based on the constructed RSM model, enabling the rapid determination of optimal design parameters. These optimized parameters are then fed back into the MC simulation model to derive the final design values. Comparative analysis with the traditional enumeration method and GA alone demonstrates the superior optimization efficiency of the proposed approach. To further validate its effectiveness, the method is applied to the optimization of a moderator-collimator system for a thermal neutron radiography system based on an accelerator. Two optimization tasks are performed: (1) determining the optimal efficiency under different source neutron energies and (2) optimization of thermal neutron photon yield ratio. The results highlight the efficiency and applicability of HRG-MCO in neutronics optimization

> Keywords: Neutronics Design Optimization, Monte Carlo Simulation, Response Surface Methodology, Genetic Algorithm, Thermal Neutron Radiography

I. INTRODUCTION

In recent years, nuclear technologies based on neutron 3 system such as advanced nuclear energy, boron neutron 4 capture therapy (BNCT) and neutron radiography have 5 developed rapidly. The advancement of these technolo-6 gies heavily relies on the design and optimization of neu-⁷ tronics [1–5]. The Monte Carlo (MC) method is widely s used in neutron system design due to its intuitive mod-9 eling and high computational accuracy [6]. However, 10 traditional MC iterative optimization methods, which 11 rely on enumeration or gradient-based approaches, re-12 quire significant expertise from designers and struggle 13 to balance multiple design factors and objectives leading 14 to optimization results that lack systematic and global efficiency [7-13]. Genetic Algorithm (GA), with its powerful multi-

parameter optimization capabilities, has been widely ap-18 plied in MC design optimization in recent years. For 20 method for estimating the parameters of typical overlap-21 ping nuclear pulse signals. First, the nuclear pulses are 22 regarded as individual genes and the norm is set as the 23 fitness function. Second, the global optimal solution is

24 found by searching the population of genetic algorithm, 25 so as to estimate the parameters of nuclear pulse [14]. 26 In 2019, Byoungil Jeon et al. proposed an optimiza-27 tion method combining genetic algorithms with MC simulations to simultaneously calculate energy calibration ₂₉ parameters and gamma response functions [15]. In the 30 same year, Guang Hu et al. optimized the structure of 31 the moderator by using the output file of the neutron en-32 ergy spectrum from MCNP5 as the objective function of 33 the GA and solving for the maximum and minimum val-₃₄ ues of the objective function through GA [16]. In 2020, 35 M.F. Yan et al. employed the genetic algorithm to opti-36 mize the structure of a fast neutron radiography system 37 [17]. In 2022, S. Bagheri applied an intelligent method 38 based on genetic algorithms, integrated with the MCNP 39 program, to optimize the radiation shielding system of 40 a small nuclear reactor, demonstrating higher optimiza-41 tion efficiency compared to traditional design methods 42 [18]. In 2023, F. Cordella et al. combined genetic algo-19 example, in 2016, Hong-Quan Huang et al. proposed a 43 rithms with MCNP6 and Geant4 for radiation shield-44 ing optimization [19]. Although the GA significantly 45 improves optimization efficiency compared to the tradi-46 tional enumeration method, its reliance on probabilistic 47 sampling, mutation, and iterative adjustments can still 48 lead to impractical computational times for large-scale, 49 high-accuracy optimization problems or those with vari-50 able boundary conditions, especially when extensive MC 51 simulations are required. Response Surface Methodol-₅₂ ogy (RSM), on the other hand, optimizes by constructing 53 multi-parameter function surface models and is currently

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[†] Corresponding author, size.chen@inest.cas.cn

₅₅ method. Due to the fast computational speed of func-₁₀₂ denotes the regression intercept; β_i , β_{ii} , and β_{ij} corre-56 tion models, RSM offers high optimization efficiency. 103 spond to the coefficients of linear, quadratic, and inter-₅₇ However, the accuracy of the RSM model construction $_{104}$ action terms, respectively; x_i and x_j are coded values of directly impacts the final optimization results [20–24]. 105 process variables; and ε accounts for residuals and ex-Therefore, building a high-accuracy RSM analysis model $_{\rm 106}$ perimental errors. is key to the successful application of the RSM method. 107 62 RSM and GA optimization techniques to establish a 109 nomials may also be considered. However, higher-order 63 more efficient neutronic design optimization method. It 110 models risk exhibiting unstable behavior in unexplored 64 is applied to the design of the moderator-collimator in 111 experimental regions and inherently require increased 65 a thermal neutron radiography system based on accel-112 computational resources to enhance prediction accuracy 66 erator, aiming to address multiple design optimization 113 [32]. The utilization of higher-order polynomials en-67 challenges encountered in the process.

II. RESEARCH METHODS

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Theory for the method

Monte Carlo simulation method

MC method is a computational technique based on

72 probability and statistics, which approximates solutions

74 ages computer simulations of stochastic processes to ob-75 tain approximate solutions [25, 26]. The primary MC 76 simulation software with neutron transport capabilities 77 includes MCNP [27], OpenMC [28], and Geant4 [29]. In this study, the Geant4 software package is em-79 ployed. Developed by CERN using C++ object oriented 128 80 technology, Geant4 is a large-scale open source software 129 optimal solutions, characterized by its ability to directly 82 cesses of various particles, including neutrons, in mat- 131 on derivatives or function continuity constraints, and exclear technology applications.

87 neutron transport, this study also employs the Gamos 136 explores solutions to complex problems. The algorithm 88 extension package compatible with Geant4 to achieve 137 maintains a diverse population and iteratively improves 89 geometry importance sampling acceleration [30].

2. Response Surface Methodology

RSM is a method that employs systematic experi- 143 92 mental design to obtain data and uses a multivariate 144 ployed to identify the extrema of the fitted function de-95 ues [31]. By analyzing the regression equation, optimal 147 bility of 0.2, and 50 iterations. The optimization process effective approach for addressing multivariate optimiza- 149 framework from the DEAP framework in Python. 98 tion problems. The multivariate quadratic regression 99 equation is expressed as:

$$y = \beta_0 + \sum_{i=1}^n \beta_i x_i + \sum_{i=1}^n \beta_{ii} x_i^2 + \sum_{i=1}^{n-1} \sum_{j=1}^n \beta_{ij} x_i x_j + \varepsilon \quad (1) \text{ The proposed method, named Hybrid of Adaptive Response Surface methodology and Genetic Algorithm}$$

 $_{54}$ another well-established multi-parameter optimization $_{101}$ —where y represents the predicted response value; β_0

While conventional RSM typically employs second-This study attempts to combine the advantages of 108 order polynomials for surface fitting, higher-order poly-114 tails a greater number of unknown coefficients and en-115 hanced functional complexity, thereby requiring meticulous evaluation of polynomial order to guarantee model 117 reliability and accuracy.

In this study, given the requirements for optimized moderator-collimator system parameters and the semi-120 automated nature of the RSM process, the computa-121 tional cost associated with implementing higher-order 122 polynomials becomes negligible compared to the sub-123 stantial resources required for MC simulations. There-124 fore, higher-order polynomial models with different or-73 to complex problems through random sampling. It lever- 125 ders are self-adopted for response surface analysis to

3. Genetic Algorithm

GA is a computer algorithm designed for searching package capable of simulating the physical transport pro- 130 manipulate structural objects, operate without reliance ter. Due to its versatility and scalability, Geant4 has 132 hibit implicit parallelism and global optimization capabeen widely applied across various fields, including nu- 133 bilities. It adaptively adjusts search directions through 134 probabilistic methods [33–35]. By simulating natural se-To further improve the computational efficiency of 135 lection and genetic variation processes, GA intelligently 138 solution quality through operations such as selection, 139 crossover, and mutation, enabling effective exploration 140 of potential optimal regions in the solution space without 141 requiring gradient information from the objective func-142 tion [36].

In this study, the genetic algorithm was primarily em- ${\rm quadratic\ regression\ equation\ to\ model\ the\ functional\ re-}^{~145}\ rived\ from\ response\ surface\ analysis,\ with\ a\ population$ lationship between influencing factors and response val- 146 size of 100, crossover probability of 0.5, mutation probaparameter combinations can be identified, making it an 148 was implemented using the classical genetic algorithm

B. Establishment of the proposed method

153 Monte Carlo Optimization (HRG-MCO), utilizes Python 204 moderation process. For the initial and model valida-154 to integrate response surface analysis algorithms, MC 205 tion phases, LHS was employed with 10 sample points in 155 calculations, and GA, with its detailed optimization de-206 each case. The stopping criterion for the response sur-156 sign workflow illustrated in Figure. 1.

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158 Sampling (LHS) to select initial calculation points with 209 flux at the point detector. the multi-dimensional design parameters. These points 160 are subsequently input into the MC model to calculate 161 the target parameters. The resulting data is then rein-162 troduced into a multi-order function to fit RSM models 163 of different orders. To validate the accuracy of the mod- $_{164}$ els, LHS is again utilized to sample test points for MC $_{210}$ 165 calculations. The relative error between the test point 211 of the RSM modeling accuracy. The results indicate predicted values from the RSM model and the MC cal- 212 that after three iterations, 100 points validation error of 167 culation values is calculated using Equation. 2 to assess the accuracy of the RSM model.

$$E = \frac{|y_1 - y_2|}{y_2} \times 100\% \tag{2}$$

Here, y_1 represents the predicted value, y_2 denotes 170 the simulated value, and \hat{E} represents the relative er- $\frac{1}{221}$ 1.640 × 10⁻⁷ for the system. 172 ror between the two. This step ensures the reliability of the constructed RSM model for subsequent optimiza-174 tion processes. When the model accuracy falls below 175 the preset accuracy criteria, the validation point data 176 is reintroduced into the multi-order function fitting pro-177 cess to enhance the accuracy of the RSM model. Subse-178 quently, new sampling points are extracted to revalidate the model accuracy. This iterative procedure is repeated until the validation accuracy of one of the response sur-181 face functions satisfies the system optimization design re-182 quirements. Based on the obtained RSM model, the GA 183 is then employed to solve the multi-parameter optimiza-184 tion problem. Finally, the optimal parameter combina-185 tion is reintroduced into the MC simulation to obtain 186 the final results of the optimized system. This approach 187 ensures a systematic and efficient optimization process 188 with high accuracy.

C. Validation of the proposed method

based on the classical optimization problem of D-T neu-239 40 samples deviates by only 0.49% from that obtained tron source moderation design to validate the effective- 240 using 40,000 samples in the enumeration method. Un-193 ness of HRG-MCO. A schematic diagram of the model 241 der identical sampling conditions, the GA results devi-194 is presented in Figure. 2. The model consists of two lay- 242 ate by 6.37% relative to the enumeration method, while 195 ers: (1) a tungsten multiplier layer with a diameter of 243 the deviation is reduced to 0.73% under the triple sam-40 cm, and (2) a polyethylene moderation layer of the 244 pling condition. These results indicate that HRG-MCO 197 same diameter. The optimization range for both lay- 245 not only achieves significantly higher optimization effi-198 ers was confined to 1-20 cm. The neutron source is set 246 ciency compared to both the enumeration method and 199 as a point source with a radius of 1 cm, positioned 20 247 GA but also maintains a high degree of computational 200 cm to the left along the central axis. A thermal neu-248 accuracy. Furthermore, as the optimization dimension 201 tron point detector was positioned at the center of the 249 increases, the growth in the number of sampling points 202 neutron exit surface of the moderation layer to record 250 further highlights the advantage of HRG-MCO in opti-

207 face model accuracy was set at 1%. The objective of the The methodology initially employs Latin Hypercube 208 GA optimization was to maximize the thermal neutron

> Figure. 3 shows the iterative computational results 213 the RSM model using a fourth-order polynomial reached 214 0.46%, which exceeds the predefined accuracy target of 215 1%. Based on this function model, the GA optimiza-216 tion was performed to determine the optimal parame-217 ters, which were identified as a neutron multiplier layer 218 thickness of 10.8 cm and a moderation layer thickness of 219 5.5 cm. Under these parameter conditions, MC simula-220 tions yielded a thermal neutron moderation efficiency of

To verify the efficiency of HRG-MCO and the accu-223 racy of its optimization results, this study compares the 224 outcomes obtained using HRG-MCO with those from the 225 enumeration approach and the classical GA method. In 226 the enumeration approach, calculations were performed 227 with a thickness interval of 0.1 cm; for GA, comparisons 228 were conducted under the same sampling conditions as $_{229}$ HRG-MCO as well as under conditions with three times 230 the sampling density. The comparative results are pre-231 sented in Figure. 4 and Table. 1. Figure. 4 illustrates 232 the comparison between the response surface model es-233 tablished by HRG-MCO (red) and that constructed via the enumeration method (blue), Where x_1 represents the $_{235}$ multiplier layer thickness and x_2 represents the moder-236 ator layer thickness, showing good consistency between 237 the two across various contour levels. Table. 1 details In this study, a two-factor MC model was established 238 that the optimal value obtained from HRG-MCO using ₂₀₃ the thermal neutron flux below 0.5 eV resulting from the ₂₅₁ mization efficiency compared to the traditional GA.

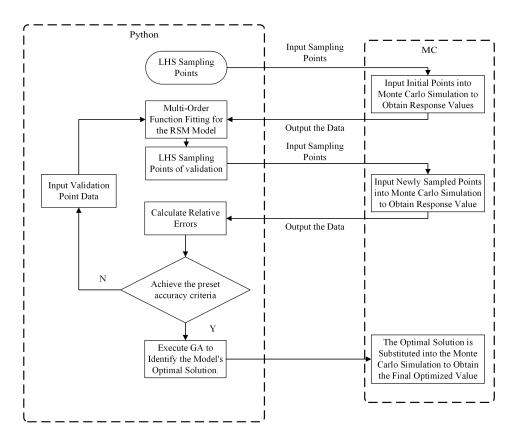


Fig. 1. Methodology flow chart of HRG-MCO.

Method	Predicted Optimal Parameter (cm)	Thermal neutron moderation efficiency	Total Number of Sampling Points	Error (Relative to Enumeration Method)
Enumeration method	[10.8, 5.5]	1.648×10^{-7}	40000	/
HRG-MCO	[10.6, 5.4]	1.640×10^{-7}	40	0.49%
GA	[7.1, 6.4]	1.543×10^{-7}	40	6.37%
GA	[10.1, 5.4]	1.636×10^{-7}	126	0.73%

APPLICATION OF THE PROPOSED METHOD IN 269 curve requires designing and optimizing the moderator-253 THERMAL NEUTRON IMAGING SYSTEMS

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255 Α. neutron energies 256

cally employ neutron sources based on an accelerator. 277 moderator-collimator is established, with the cylindrical 259 Depending on the specific neutron-producing reaction 278 structure. Figure. 5 shows a cross-sectional view along channels or the accelerator beam energy, the energy of 279 the central axis, where the yellow region represents the the source neutrons can be adjusted as required. Since 280 heavy metal multiplication layer, the green region repthe different source neutron energies will directly affect 281 resents the polyethylene moderator layer, and the blue the thermal neutron moderation efficiency of the mod-282 region represents the graphite reflector. The inner wall of erator collimator, determining the optimal moderation 283 the collimation channel is lined with a 1-mm thick therefficiency at different neutron energies is crucial for se-284 mal neutron shielding layer, while the outermost layer of 266 lecting the neutron source and accelerator beam energy 285 the moderator-collimator is a 10-mm thick BC₄ thermal 267 in neutron radiography systems. However, under tradi- 286 shield. In line with Section 2.3, a thermal neutron point

 ${\rm MODERATOR\text{-}COLLIMATOR\ DESIGN\ FOR\ COMPACT}_{\rm\ 270}\ collimator\ for\ each\ individual\ energy\ point.\ This\ process$ ²⁷¹ makes it challenging to rapidly generate such a curve and 272 even more challenging to conduct a quantitative assess-Study on moderation efficiency under different incident 273 ment of the impact of various heavy metal multiplier 274 materials on the optimal moderation efficiency curve.

275 To address the above issues, we conducted relevant Compact thermal neutron radiography systems typi- 276 research using HRG-MCO. First, an MC model of the 268 tional methods, obtaining the neutron energy efficiency 287 detector is placed at a collimation ratio (L/D) of 10. A

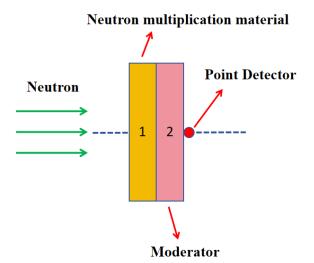


Fig. 2. (Color online) Structural diagram under two factors. 320

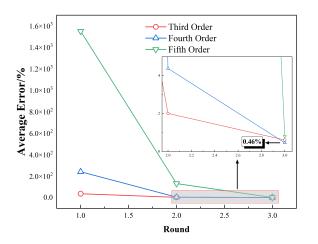


Fig. 3. (Color online) The relationship between the number method validation.

289 the left entrance of the collimator. To enhance the gen- 343 and depleted uranium (DU), the optimal moderation ef-290 eral applicability of this research, no specific accelerator 344 ficiency curves of Pb and DU were calculated using the ₂₉₁ target room was modeled. Instead, the neutron source ₃₄₅ aforementioned methodology, with the comparative re-292 is defined as a planar source with a diameter of 20 mm, 346 sults illustrated in Figure. 8. The optimized parameters 293 placed perpendicular to the moderator-collimator axis 347 of each material layer were systematically compared in 294 on the left side of the multiplication layer. In the figure, 348 Figure. 9. As clearly demonstrated in Figure. 8, DU ex-295 the parameters labeled 1 through 4 correspond to four 349 hibits significantly superior moderation efficiency com-296 optimization variables of the model: (1) the thickness of 350 pared to the other two materials. Figures . 9(a) and 297 the front neutron multiplication layer, (2) the thickness 351 . 9(b) reveal that the enhanced performance of DU priof the outer neutron multiplication layer, (3) the thick- 352 marily stems from its lower energy threshold for neutron 299 ness of the polyethylene moderator layer, and (4) the 353 multiplication, enabling effective neutron generation at 300 energy of the source neutrons. Since achieving the mini- 354 lower energy levels. Furthermore, Figure. 9(c) shows 301 mum neutron leakage rate would theoretically require an 355 that the average energy of fast neutrons generated by DU 302 infinitely thick reflector and considering practical design 356 and W multiplication is lower than that of Pb, indicat-303 constraints, the radial graphite reflector thickness is ar- 357 ing that a smaller moderator layer thickness is beneficial 304 tificially set at 20.0 cm, while the axial graphite reflector 358 for improving neutron moderation efficiency.

305 thickness in the collimation zone is set at 39 cm.

For the design optimization calculation, both the ini-307 tial LHS sampling and the verification sampling were performed with a sample size of 100 points, and the RSM model verification accuracy was set to 5%. Fig-310 ure. 6 shows the final iterative calculation results for the RSM modeling verification accuracy. It can be ob-312 served that after five iterations, the verification accuracy of the eighth-order polynomial fit reached 4.96%, thereby 314 achieving the targeted accuracy.

In order to obtain the optimal curve of neutron moderating efficiency varying with energy, different energy values were successively introduced into the established RSM model function at 0.5 MeV intervals within the 1-14 MeV energy region as the fitness function of GA optimization for each energy point. Then GA and MC methods were used to obtain the optimal design parameters and efficiency values for each energy point. Figure. 7 illustrates the variation in optimal moderation efficiency with energy (a) and the corresponding values of three optimized parameters (b) when W is used as multiplication material. It can be observed that in the 1-14 MeV energy range, the overall trend of the optimal thermal neutron moderation efficiency is a decrease followed by an increase as the incident neutron energy rises. A further comparison of the data trends in the two graphs reveals that the outer neutron multiplication layer becomes effective at lower source neutron energies compared to the 333 forward neutron multiplication layer; however, the outer 334 layer merely slows the rate of decline in thermal neutron 335 moderation efficiency. In contrast, although the forward 336 neutron multiplication layer only becomes active in the 337 energy region above 6 MeV, its impact on thermal neu-338 tron moderation efficiency is significant. With the incorof iterations and the average error of each order model in 339 poration of the forward neutron multiplication layer, the 340 thermal neutron moderation efficiency quickly increases.

To comparatively investigate the performance differ-288 mounting space for the accelerator target is reserved at 342 ences among multiplier layer materials including Pb, W,

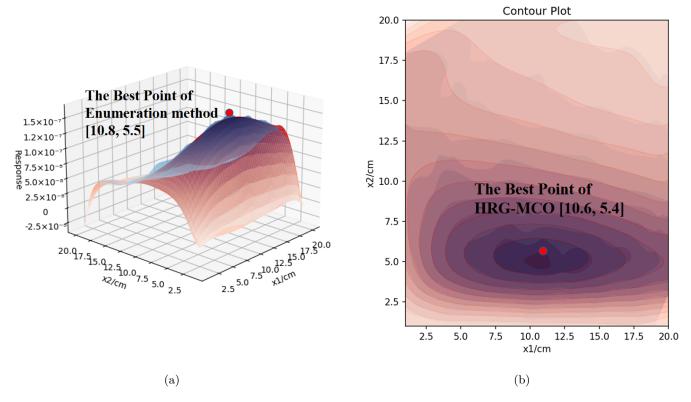
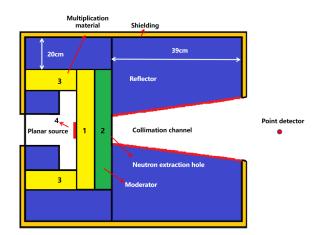
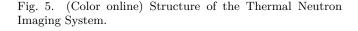


Fig. 4. (Color online) (a) Three-dimensional response surface plot and (b) corresponding contour plot derived from two-factor validation and simulations.





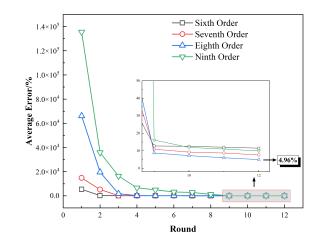


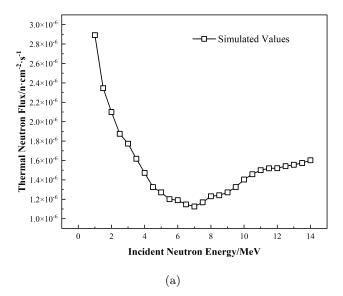
Fig. 6. (Color online) Results of RSM model accuracy verification in the energy optimal moderation efficiency problem.

B. Optimization of thermal neutron photon yield ratio

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cal imaging system is the most commonly used imaging 370 sign optimization objective for the moderator-collimator 362 scheme in thermal neutron radiography systems. Due 371 system in accelerator-based thermal neutron radiogra-363 to the high energy of the neutrons in the accelerator 372 phy. However, an intrinsic trade-off exists between ther-364 source, the imaging quality is not only related to the 373 mal neutron flux and photon yield ratio: increasing 365 emitted thermal neutron flux but also inevitably affected 374 the photon yield ratio requires incorporating more high-366 by the leakage of high-energy neutrons, which leads to 375 energy neutron-absorbing materials, but their excessive

367 the deterioration of imaging resolution. Therefore, max-368 imizing the proportion of thermal neutron-induced pho-The combination of a conversion screen and an opti- 369 ton yield in the conversion screen is another critical de-



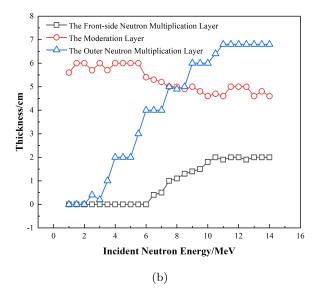


Fig. 7. (Color online) (a) Variation curve of optimal moderation efficiency with energy; (b) Relationship between incident neutron energy and thickness parameters of key components.

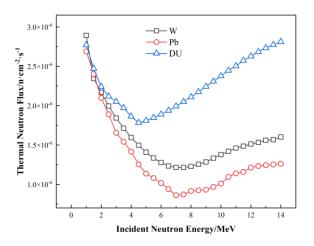


Fig. 8. (Color online) The variation curve of optimal moderation efficiency with energy for various multiplier materials.

 $_{376}$ use can negatively impact the transport efficiency of $_{412}$ 377 thermal neutrons. Using the newly developed optimiza- 413 fitness function was constructed as explicitly defined in 378 tion method, we investigate the photon yield optimiza- 414 Equation. 3: tion problem based on a D-T neutron source thermal neutron radiography model to enhance the performance of the imaging system.

Figure. 10(a) shows the variation curve of the photon yield of the ⁶LiF/ZnS thermal neutron conversion screen 384 as a function of neutron energy, as obtained from the au-385 thors' previous research [37]. Based on this curve, the 416 386 impact of neutrons at different energy levels on photon 387 yield can be assessed using the neutron energy spectrum 417 388 from MC simulations of the moderator. As a prelim-389 inary study, to enhance computational efficiency, neu-390 tron energy is categorized into four energy regions: the 418 391 thermal neutron region, epithermal neutron region, res-

392 onance neutron region, and fast neutron region, which ³⁹³ are delineated in Figure. 10(a) with vertical dashed lines. The MC model adopts the same geometric configuration 395 as in Figure. 5, with the neutron source energy fixed at 14.1 MeV from a D-T neutron source. W, a readily available material with moderate performance, is selected as the metal neutron multiplication layer. The thermal neutron point detector is replaced with a full-spectrum point detector, which records the flux proportions of neutrons emitted from the moderator-collimator within the four defined energy regions. The decision variables remain 403 consistent with the first three variables in Section 3.1: 404 the thickness of the front neutron multiplication layer $_{405}$ (x_1) , the thickness of the outer neutron multiplication 406 layer (x_2) , and the thickness of the polyethylene moderator layer (x_3) . Figure. 10(b) illustrates the accuracy validation of the high-order RSM function. The results 409 indicate that after three iterations, the sixth-order model 410 is the first to meet the predefined 3% accuracy validation 411 criterion.

To optimize the thermal neutron proportion, a GA

$$F_5 = \frac{w_1 F_1}{w_1 F_1 + w_2 F_2 + w_3 F_3 + w_4 F_4} \tag{3}$$

$$\max F(x_1, x_2, x_3) = \begin{cases} \max F_1(x_1, x_2, x_3) \\ \max F_5(F_1, F_2, F_3, F_4) \end{cases}$$

subject to
$$\begin{cases} 0 < x_1 \le 20 \\ 0 < x_2 \le 20 \\ 0 < x_3 \le 20 \end{cases}$$
 (4)

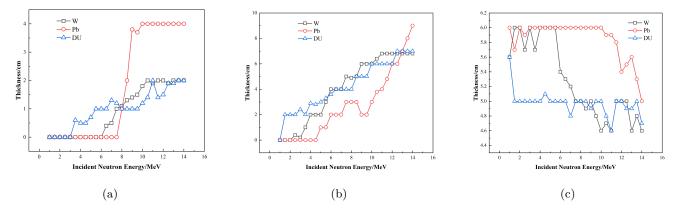


Fig. 9. (Color online) Comparison of optimized parameters for three multiplier materials: (a) front-side multiplier layer optimization, (b) outer multiplier layer, and (c) moderation layer.

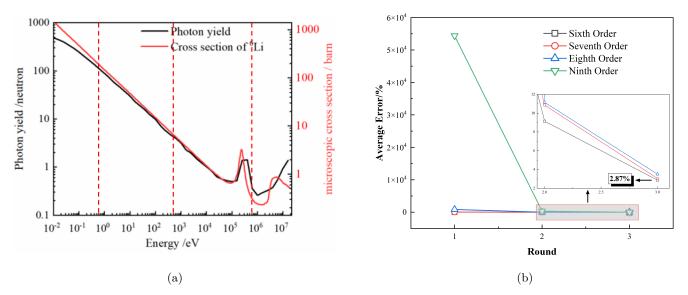


Fig. 10. (Color online) (a) Relationship between photon yield and neutron energy [37] and (b) Accuracy verification results of the RSM modeling for the light yield optimization of the moderator-collimator system.

In the equation, F_5 represents the function that de- 430 pressed in Equation. 4: $_{420}$ scribes the proportion of thermal neutron photon yield $_{431}$ In this equation, F represents the overall objective w_1 relative to the total photon yield. The coefficients w_1 w_2 function, with the optimization space for decision vari w_4 correspond to the photon yield weights of ther- w_4 ables w_4 to w_4 constrained to the range of 0 to 20 cm. 423 mal neutrons, epithermal neutrons, resonance neutrons, 434 The parameters for the GA are set as follows: the parent and fast neutrons, respectively, as determined from Fig- $_{435}$ population size (μ) is 100, the offspring population size ure. 10(a) and detailed in Table. 2. F_1 to F_4 represent $_{436}$ (λ) is 200, the crossover probability is 0.5, the mutation 426 the neutron flux rates in the four energy regions, calcu- 437 probability is 0.2, and the maximum number of genera-427 lated using the established RSM functions.

TABLE 2. Weighting factors for light yield across different $^{440}\,$ energy regions.

Energy Region	W_1	W_2	W_3	W_4
Energy Region	(Thermal)	(Epithermal)	(Resonance)	(Fast)
Average Value	368.29	35.69	1.43	0.56
Normalization	0.907	0.088	0.004	0.001

429 function for NSGA-II can be further established, as ex-448 when the photon yield ratio is below 90%, the decline in

438 tions is 100. A blended crossover operator is employed, 439 and Gaussian mutation is applied to balance solution diversity and convergence.

Figure. 11 presents the Pareto front solutions obtained 442 through GA optimization. As shown in Figure. 11, a 443 nonlinear inverse relationship exists between the optimal 444 solutions of thermal neutron flux and its photon yield ra-445 tio. As the thermal neutron flux increases, the photon 446 yield ratio decreases gradually. By analyzing the slope Building on Equation. 3, the optimization constraint 447 variation of the relationship curve, it is observed that

449 thermal neutron flux due to an increase in the photon 467 450 yield ratio is relatively gradual. However, once the pho- $_{451}$ ton yield ratio exceeds 90%, the decline rate of thermal $_{468}$ 452 neutron flux accelerates significantly.

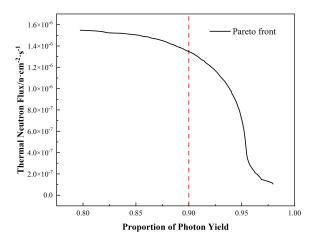


Fig. 11. (Color online) Pareto optimal solution sets.

The model parameters at a photon yield ratio of 90% $_{454}$ ($x_1 = 3.8$ cm, $x_2 = 5.6$ cm, $x_3 = 19.4$ cm) were substi-455 tuted into the MC model to recalculate the correspond-456 ing neutron energy spectrum, as shown in Figure. 12(a). $_{457}$ Based on this spectrum, the photon yield distribution $_{501}$ 458 as a function of neutron energy was further computed, $_{459}$ as illustrated in Figure. 9(b). The results indicate that $_{502}$ $_{460}$ non-thermal neutrons account for the largest proportion $_{503}$ newly developed multi-objective parameter optimization of the total neutron flux, reaching 61.9%. However, their 504 method exhibits high design efficiency and accuracy in $_{462}$ contribution to photon production is minimal, making $_{505}$ addressing multi-parameter optimization problems for $_{463}$ up only 0.61%. In contrast, although thermal neutrons $_{506}$ the design of thermal neutron radiography moderator- $_{464}$ represent only 8.2% of the total flux—less than a quar- $_{507}$ collimators. Further validation and application in other $_{465}$ ter of the total—they contribute up to 90.1% of the total $_{508}$ neutronics fields, such as BNCT, will be conducted in 466 photon yield.

CONCLUSION

This study proposes a novel neutronics optimization 469 design method that adaptively constructs a multi-order 470 function model using RSM based on MC simulation 471 results, followed by GA optimization. The proposed 472 approach is applied to the design optimization of a moderator-collimator system for thermal neutron radiography. The key research findings are listed below:

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- 1. By comparing the optimization results of HRG-MCO with those of the enumeration method and the traditional GA method for the neutron moderation problem of bilayer materials, the deviation of the results obtained using 40 sample points is only 0.49% compared to those obtained using 40,000 sample points in the enumeration method. Additionally, HRG-MCO outperforms the GA in optimization results under both the same sampling conditions and three times the sampling density.
- 2. An investigation of neutron moderation efficiency under varying incident neutron energies reveals that in the energy range of 1–14 MeV, the optimal moderation efficiency of the moderator-collimator initially decreases and then increases. Moreover, the efficiency ranking of W, Pb, and DU as neutron multiplication materials follows the order: DU > W > Pb.
- 3. Optimization of the conversion screen photon yield in a D-T neutron source-based thermal neutron radiography system reveals a nonlinear trade-off between thermal neutron flux and thermal neutron photon yield ratio. When the photon yield ratio exceeds 90%, the thermal neutron flux experiences a significant decline. At a photon yield ratio of 90%, the thermal neutron flux reaches approximately 85% of its maximum value.

The results of the above study demonstrate that the 509 the following study.

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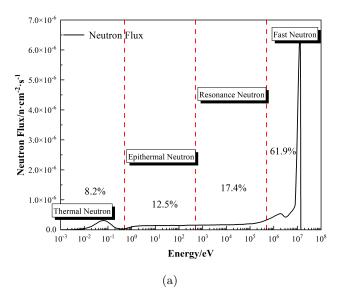
517

^[1] Y.N. Zhu, Z.K. Lin, H.Y. Yu et al., "Study on the op- 518 timal incident proton energy of ⁷Li(p, n) ⁷Be neutron 519 source for boron neutron capture therapy," Nucl. Sci. 520 Tech. 35, 60 (2024). doi: 10.1007/s41365-024-01420-6.

Y. Zhang, C. Liu, S.L. Liu et al., "Prompt fission neu- 522 tron uranium logging (II): dead-time effect of the neu- 523 tron time spectrum," Nucl. Sci. Tech. 36, 19 (2025). doi: 524 10.1007/s41365-024-01615-x.

^[3] Z.P. Qiao, Y.C. Hu, Q.X. Jiang et al., "Coin-structured tunable beam shaping assembly design for acceleratorbased boron neutron capture therapy for tumors at different depths and sizes," Nucl. Sci. Tech. 34, 186 (2023). doi: 10.1007/s41365-023-01325-w.

Y. Kiyanagi, "Neutron applications developing at compact accelerator-driven neutron sources," AAPPS Bull. 31, 1 (2021): 22.



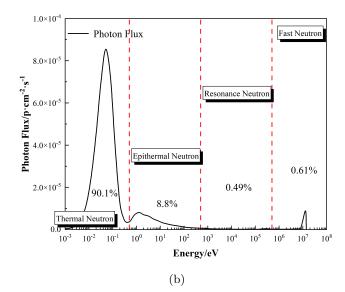


Fig. 12. (Color online) (a) Neutron fluence rates across different energy intervals and (b) Photon yield distribution.

584

[5] Y. Sun, Q.B. Wang, P.C. Li et al., "Indirect neutron 566 radiography experiment on dummy nuclear fuel rods for 567 pressurized water reactors at CMRR," Nucl. Sci. Tech. 568 35, 189 (2024). doi: 10.1007/s41365-024-01534-x.

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- P.F. Shen, X.D. Huo, Z.G. Li et al., "Mesh-free 570 semi-quantitative variance underestimation elimination 571 [16] method in Monte Carlo algorithm," Nucl. Sci. Tech. 34, 572 14 (2023). doi: 10.1007/s41365-022-01156-1.
- Bai X., Ma J., Wei Z., et al., Development of a high-yield 574 [7] compact DD neutron generator. Nuclear Instruments 575 and Methods in Physics Research Section A: Acceler- 576 ators, Spectrometers, Detectors and Associated Equip- 577 ment 2024, 169993.
- Iverson E. B., Enhancing neutron beam production with 579 a convoluted moderator. Nucl. Instrum. Methods Phys. 580 Res. Sect. A 762, 31–41 (2014).
- de Haan V., A high performance neutron moderator de- 582 sign. Nucl. Instrum. Methods Phys. Res. Sect. A 794, 583 122-126 (2015).
- Schönfeldt T., Advanced Neutron Moderators for the 585 545 ESS (2016).
- Prastowo D., Design of Neutron Activation and Ra- 587 547 548 diography Facilities Based on DD Generator. In- 588 donesian Journal of Physics 34(2), 1-7 (2023). doi: 589 $10.5614/\mathrm{itb.ijp.} 2023.34.2.1$ 550
- Li C., Jing S., Gao Y., Zhang W., MCNP optimization of 591 551 fast neutron beam thermalization device based on D-T 592 552 neutron generator. Fusion Engineering and Design 151, 593 553 111385 (2020). doi: 10.1016/j.fusengdes.2019.111385 554 594
- Li H., et al., Design of moderator and collimator for com- 595 [23] 555 pact neutron radiography systems. Nuclear Instruments 596 and Methods in Physics Research Section A: Acceler- 597 ators, Spectrometers, Detectors and Associated Equip- 598 ment 959, 163535 (2020).
- H.Q. Huang, X.F. Yang, W.C. Ding et al., "Estimation 600 560 method for parameters of overlapping nuclear pulse sig- 601 [24] nal," Nucl. Sci. Tech. 28, 12 (2017). doi: 10.1007/s41365-602 562 016-0161-z.
- Jeon B., Kim J., Moon M., Cho G., Parametric op- 604 564 [15] timization for energy calibration and gamma response 605 565

- function of plastic scintillation detectors using a genetic algorithm. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 930 (2019). doi: 10.1016/j.nima.2019.03.003
- Hu G., et al., A novel method for designing the moderator of accelerator-driven neutron source. Annals of Nuclear Energy 133, 96-99 (2019).
- Yan M. F., et al., Optimization design of a fast neutron imaging collimator by genetic algorithm. Journal of Instrumentation 15(12), P12002 (2020).
- Bagheri S., Khalafi H., SMR, 3D source term simulation for exact shielding design based on genetic algorithm. Annals of Nuclear Energy 191, 109915 (2023). doi: 10.1016/j.anucene.2023.109915
- Cordella F., Cappelli M., Ciotti M., et al., Genetic algorithm for multilayer shield optimization with a custom parallel computing architecture. Eur. Phys. J. Plus 139, 150 (2024). doi: 10.1140/epjp/s13360-023-04842-0
- [20] Lamidi S., et al., Applications of response surface methodology (RSM) in product design, development, and process optimization. IntechOpen (2022).
- [21]Sahoo P., Optimization of turning parameters for surface roughness using RSM and GA. Advances in Production Engineering & Management 6(3) (2011).
- Baligidad S. M., et al., RSM optimization of parameters influencing mechanical properties in selective inhibition sintering. Materials Today: Proceedings 5(2), 4903-4910 (2018).
- Ahmad A., Yadav A. K., Singh A., Process optimization of spirulina microalgae biodiesel synthesis using RSM coupled GA technique: a performance study of a biogas-powered dual-fuel engine. International Journal of Environmental Science and Technology 21(1), 169-188 (2024).
- Rahimi G., Chirlesan D., Soltani Z., Optimization of filler content and minimizing thickness of polymeric composite for shielding against neutron source by Response Surface Methodology (RSM) and Monte Carlo simulation. The European Physical Journal Special Topics

232(10), 1657-1663 (2023).

606

- 607 [25] Lux I., Monte Carlo Particle Transport Methods. CRC 629
 608 Press (1991). doi: 10.1201/9781351074834
 630
- ⁶⁰⁹ [26] Z.P. Chen, A.K. Sun, J.C. Lei et al., "Multi-function and ⁶³¹ generalized intelligent code-bench based on Monte Carlo ⁶³² method (MagicMC) for nuclear applications," Nucl. Sci. ⁶³³ [33]
 ⁶¹² Tech. 36, 57 (2025). doi: 10.1007/s41365-024-01626-8. ⁶³⁴
- 613 [27] Briesmeister J. F., MCNP-A general purpose Monte 635 614 Carlo code for neutron and photon transport. Manual 636 615 Version C (1986).
- 616 [28] Romano P. K., Horelik N. E., Herman B. R., et al., 638
 617 OpenMC: A state-of-the-art Monte Carlo code for re- 639 [35]
 618 search and development. Annals of Nuclear Energy 82, 640
 619 90-97 (2015). doi: 10.1016/j.anucene.2014.07.048
 641 [36]
- 620 [29] Agostinelli S., et al., GEANT4—a simulation toolkit. 642
 Nuclear Instruments and Methods in Physics Research 643
 622 Section A 506(3), 250-303 (2003).
- [30] P. Arce, F. Sansaloni and J. Lagares, "Point Detector Scorer in GAMOS/Geant4," IEEE Nuclear Science 646
 Symposium & Medical Imaging Conference, Knoxville, 647
 TN, USA, 2010, pp. 1182-1184. doi: 10.1109/NSS-MIC.2010.5873954.

[31] D.C. Montgomery, Design and analysis of experiments. Wiley, 2017.

628

- [32] M.R. Rajashekhar, "A new look at the response surface approach for reliability analysis," Struct. Saf. 12, 3 (1993): 205-220.
- [33] Z. Michalewicz and C.Z. Janikow, "GENOCOP: a genetic algorithm for numerical optimization problems with linear constraints," Commun. ACM 39, 12es (1996): 175-es.
- [34] L. Davis, Genetic algorithms and simulated annealing, 1987.
- [35] J.R. Sampson, Adaptation in natural and artificial systems (John H. Holland), 1976.
- [36] K. Deb et al., "A fast and elitist multiobjective genetic algorithm: NSGA-II," IEEE Trans. Evol. Comput. 6, 2 (2002): 182-197.
- L.X. Zhang, S.Z. Chen, Z.D. Zhang et al., "Resolution analysis of thermal neutron radiography based on accelerator-driven compact neutron source," Nucl. Sci.
 Tech. 34, 76 (2023). doi: 10.1007/s41365-023-01227-x.